IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.60 HI60

This datasheet last evaluated: June 2015; last change in preferred values: June 2015

$CF_3CF_2CH_2OH$ + ice
$CF_3CF_2CF_2CH_2OH$ + ice

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
Partitioning coefficients: K_{linC}/cm			
pentafluopropanol-1			
150 ±33	203	Moreno et al., 2012	CWFT-MS (a)
46.4 ±11.6	210		
27.5 ±5	217		
12.6 ±2	223		
heptafluobutanol-1		Moreno et al., 2012	CWFT-MS (a)
295 ± 67	203		
108 ± 36	210		
57 ± 9	217		
24.5 ± 3.4	223		

Comments

(a) Uptake of $CF_3CF_2CH_2OH$ (2,2,3,3,3 pentafluopropanol-1) and $CF_3CF_2CF_2CH_2OH$ (2,2,3,3,4,4,4 heptafluopropanol-1) on a surface film formed by freezing liquid water on inner wall of flow tube. Concentration The adsorption was fully reversible and the data could be described in terms of the Langmuir isotherm over the temperature range 203–223 K. Analysis of the isotherm for gave N_{max} = (2.9 ± 0.4) x 10^{14} molecule cm^{-2} for $CF_3CF_2CH_2OH$ and (3.0 ± 0.5) x 10^{14} molecule cm^{-2} for $CF_3CF_2CF_2CH_2OH$, independent of temperature. The cited K_{linC} values were obtained from the product $K_{LangC}(T)$ x N_{Max} (= K_{linC}) at each temperature which was within 5% of the slope of the linearised Langmuir plots at the lower concentrations. The temperature dependence of the dimensionless adsorption enthalpy gave ΔH_{ads} = (-45 ± 11) $kJmol^{-1}$ for $CF_3CF_2CH_2OH$ and ΔH_{ads} = (-46 ± 16) $kJmol^{-1}$ for $CF_3CF_2CF_2CH_2OH$ (error is 2σ + 5%).

Preferred Values

$CF_3CF_2CH_2OH$ and $CF_3CF_2CF_2CH_2OH$

Parameter	Value	T/K
K_{linC} / cm	4.2 x 10^{-10} exp(5390/T)	203 -228
N_{max} / molecule cm^{-2}	2.8 x 10^{14}	203 -228
K_{linC} / cm	4.2 x 10^{-10} exp(5390/T)	203 -228
N_{max} / molecule cm^{-2}	2.8 x 10^{14}	203 -228

Reliability		
$\Delta(E/R)$ / K	± 1000	200 - 230
ΔN_{max}	± 0.5 x 10^{14}	223 - 231

Comments on Preferred Values

The studies of and Moreno et al.(2012a) are the only data reported for the longer chain fluoroalcohols. The uptakes were fully reversible and the Langmuir contants were of similar magnitude to CF_3CH_2OH, reported in an earlier study (Moreno et al (2012b) on pure ice, which was in agreement with results of Symington et al. (2012). The preferred values accept the values of Moreno et al. (2012).

References

Moreno, E., Aranda, A., Dıaz-de-Mera, Y., Martınez, E., Bravo, I. and Rodrıguez, D., Phys. Chem. Chem. Phys., 14, 4425, 2012b.

Moreno, E., Aranda, A., Dıaz-de-Mera, Y., Notario.A, Rodrıguez, and A. Bravo, I., Atmos.Environment, 60, 76, 2012a.

Symington, A., Leow, Lay May, Griffiths, P.T., and Cox, R.A., J.Phys.Chem. A, 116, 5990, 2012

Fig 1 Temperature dependence of K_{linC} for uptake of CF_3CH_2OH on ice